



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:53 PM UTC

PDB ID : 5WXU / pdb_00005wxu
Title : 11S globulin from Wrightia tinctoria reveals auxin binding site
Authors : Kumar, P.; Kesari, P.; Dhindwal, S.; Kumar, P.
Deposited on : 2017-01-09
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

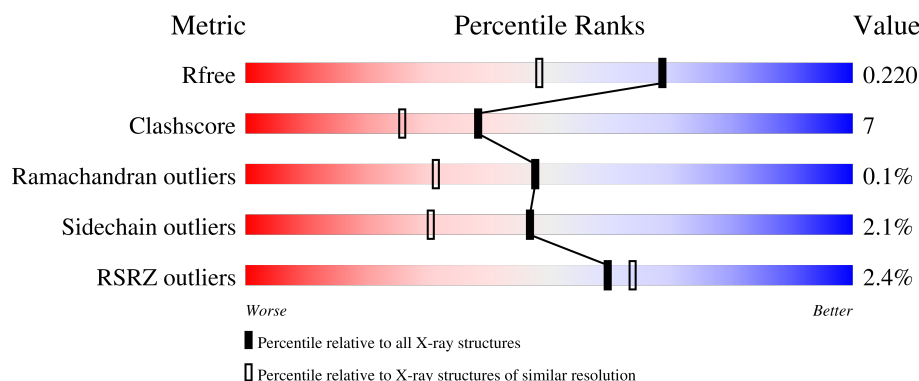
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	479	0% 73% 9% 17%
1	B	479	3% 71% 12% 16%
1	C	479	2% 72% 10% 17%
1	D	479	3% 72% 9% 17%
1	E	479	2% 72% 10% 17%

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Mol	Chain	Length	Quality of chain
1	F	479	 % 72% 10% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	B	501	-	X	-	-
3	FLC	A	503	-	X	X	-
3	FLC	B	504	-	X	-	-
3	FLC	C	501	-	X	X	-
3	FLC	D	502	-	X	-	-
3	FLC	E	504	-	X	-	-
3	FLC	F	501	-	X	-	-
4	GOL	B	503	-	X	-	-
6	PEG	D	505	-	-	X	-
6	PEG	E	506	-	-	X	-
6	PEG	F	505	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21977 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 11S globulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	20	0
			3360	2102	620	631	7			
1	B	400	Total	C	N	O	S	0	12	0
			3281	2060	600	614	7			
1	C	397	Total	C	N	O	S	0	9	0
			3240	2035	595	603	7			
1	D	396	Total	C	N	O	S	0	4	0
			3192	2006	584	595	7			
1	E	397	Total	C	N	O	S	0	6	0
			3221	2020	590	604	7			
1	F	398	Total	C	N	O	S	0	10	0
			3264	2047	599	610	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	GLN	ARG	conflict	UNP A0A162EGL7
A	459	ASP	GLY	conflict	UNP A0A162EGL7
B	147	GLN	ARG	conflict	UNP A0A162EGL7
B	459	ASP	GLY	conflict	UNP A0A162EGL7
C	147	GLN	ARG	conflict	UNP A0A162EGL7
C	459	ASP	GLY	conflict	UNP A0A162EGL7
D	147	GLN	ARG	conflict	UNP A0A162EGL7
D	459	ASP	GLY	conflict	UNP A0A162EGL7
E	147	GLN	ARG	conflict	UNP A0A162EGL7
E	459	ASP	GLY	conflict	UNP A0A162EGL7
F	147	GLN	ARG	conflict	UNP A0A162EGL7
F	459	ASP	GLY	conflict	UNP A0A162EGL7

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



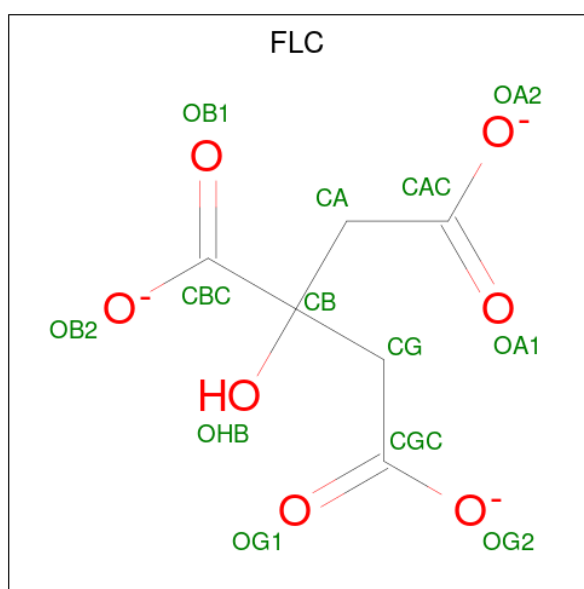
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



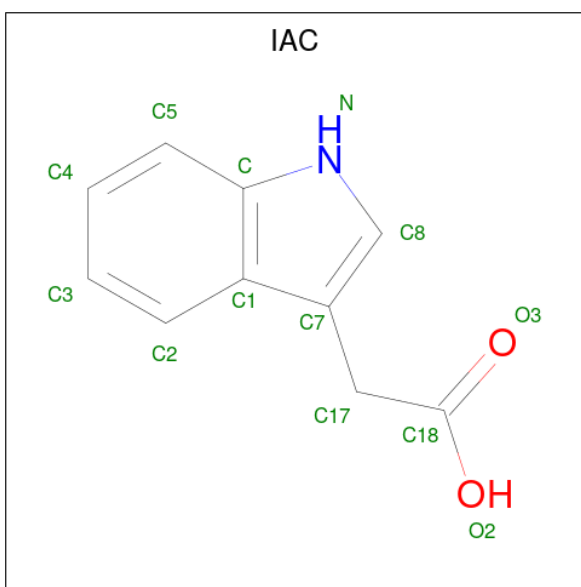
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		
3	E	1	Total	C	O	0	0
			13	6	7		
3	F	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



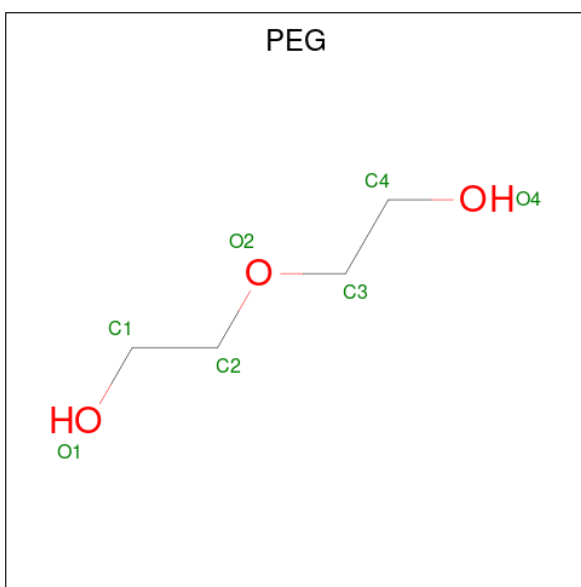
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 1H-INDOL-3-YLACETIC ACID (CCD ID: IAC) (formula: C₁₀H₉NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			26	20	2	4		
5	B	1	Total	C	N	O	0	1
			26	20	2	4		
5	D	1	Total	C	N	O	0	1
			26	20	2	4		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			7	4	3		
6	F	1	Total	C	O	0	0
			7	4	3		

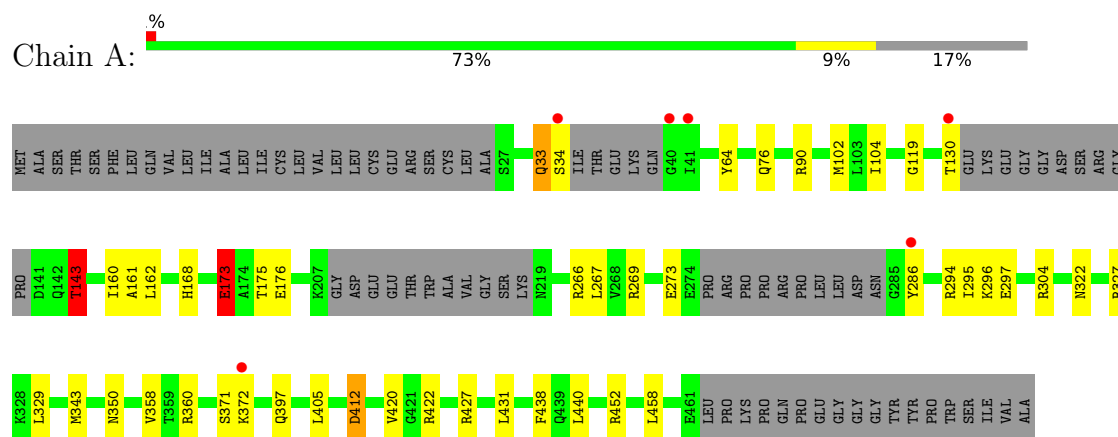
- Molecule 7 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	388	Total	O		0	0
			388	388			
7	B	346	Total	O		0	0
			346	346			
7	C	327	Total	O		0	0
			327	327			
7	D	339	Total	O		0	0
			339	339			
7	E	352	Total	O		0	0
			352	352			
7	F	346	Total	O		0	0
			346	346			

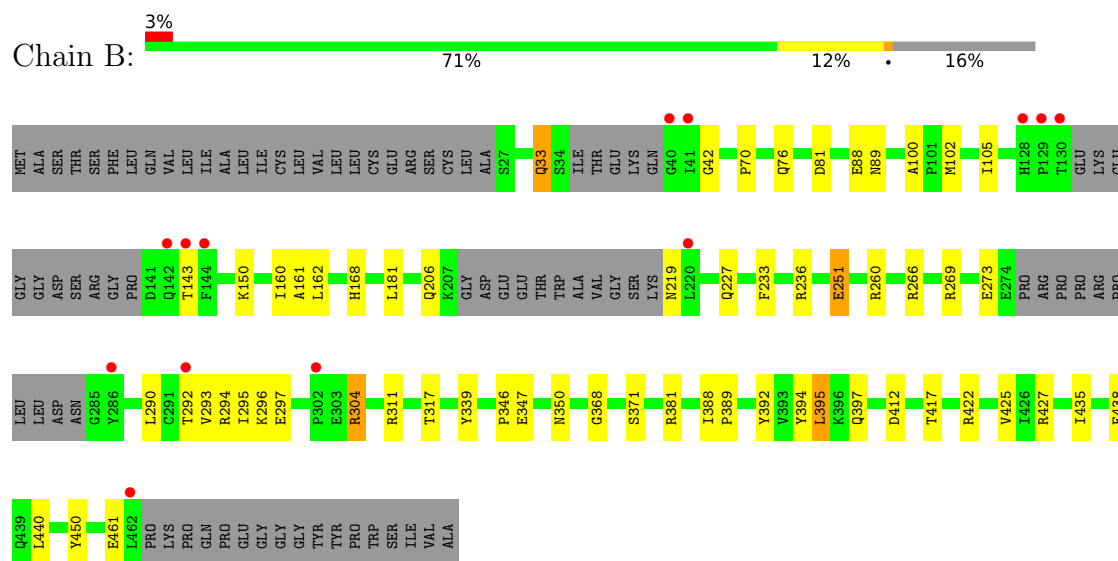
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 11S globulin

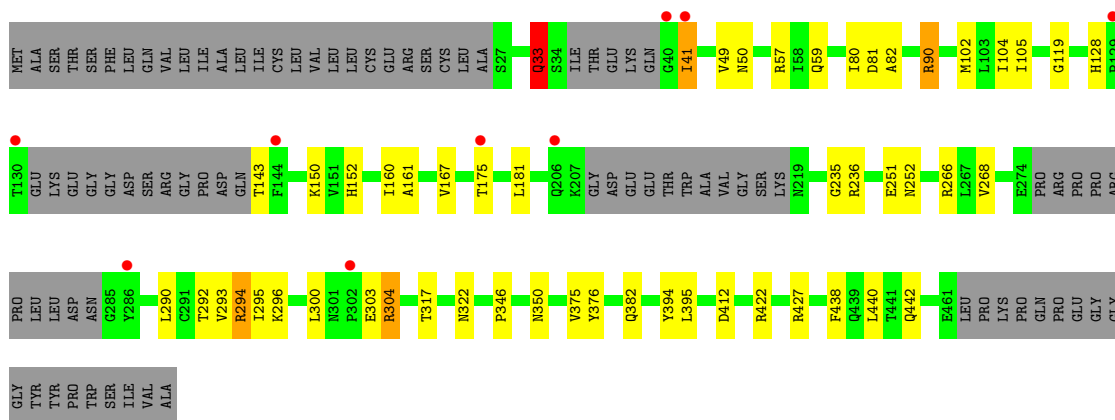


• Molecule 1: 11S globulin

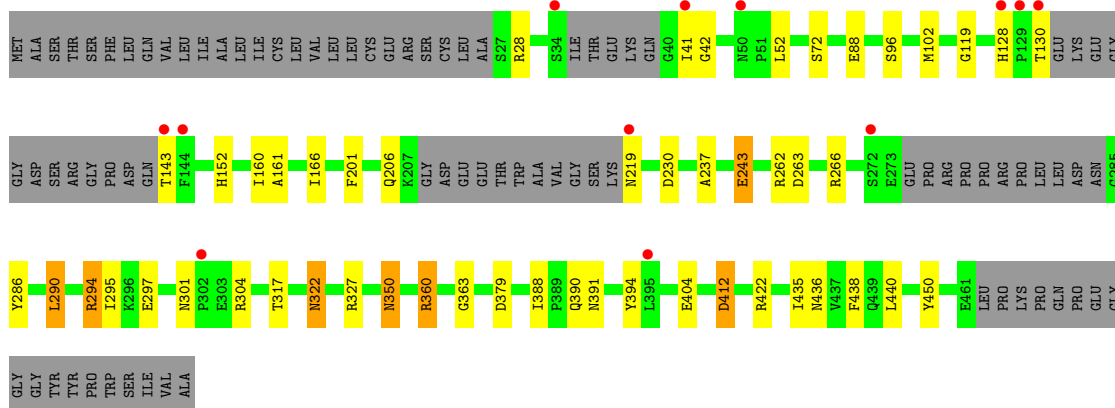
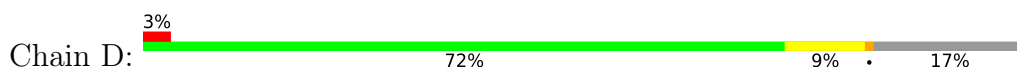


• Molecule 1: 11S globulin

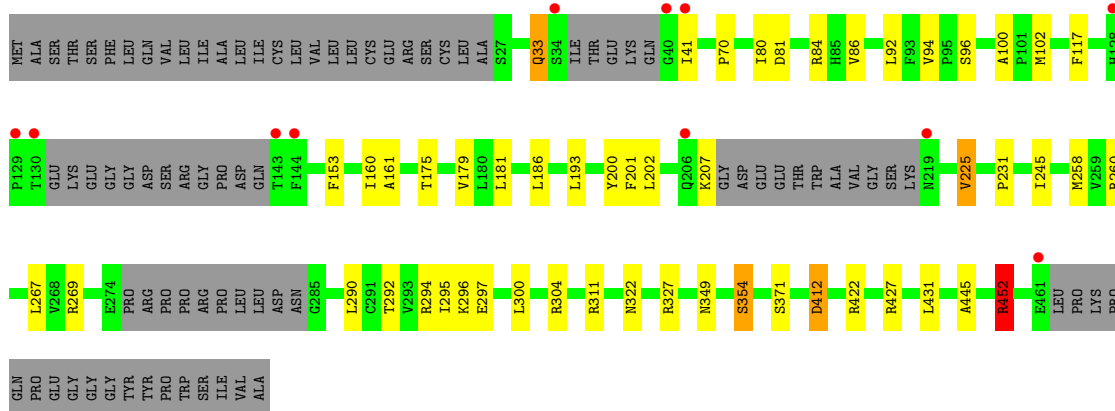




• Molecule 1: 11S globulin

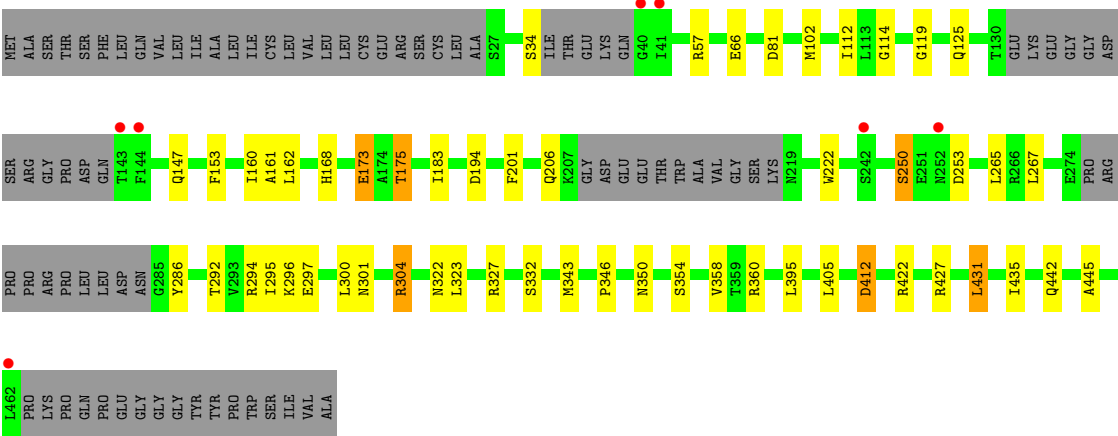


• Molecule 1: 11S globulin



• Molecule 1: 11S globulin





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.21Å 114.24Å 202.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.24 – 1.70 101.24 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.2 (101.24-1.70) 75.1 (101.24-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.174 , 0.227 (Not available) , 0.220	Depositor DCC
R_{free} test set	13476 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21977	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PEG, FLC, PO4, IAC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.24	3/3425 (0.1%)	1.11	3/4641 (0.1%)
1	B	1.31	9/3360 (0.3%)	1.16	6/4556 (0.1%)
1	C	1.32	9/3316 (0.3%)	1.17	3/4495 (0.1%)
1	D	1.30	3/3259 (0.1%)	1.16	6/4420 (0.1%)
1	E	1.31	9/3285 (0.3%)	1.16	3/4454 (0.1%)
1	F	1.30	12/3328 (0.4%)	1.14	8/4512 (0.2%)
All	All	1.30	45/19973 (0.2%)	1.15	29/27078 (0.1%)

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	412[A]	ASP	C-O	9.61	1.35	1.23
1	C	412[B]	ASP	C-O	9.61	1.35	1.23
1	E	100	ALA	CA-C	-7.68	1.45	1.52
1	A	412	ASP	C-O	7.38	1.32	1.23
1	F	412	ASP	N-CA	-7.19	1.36	1.46
1	F	435	ILE	N-CA	6.96	1.54	1.46
1	C	394	TYR	CA-C	-6.81	1.44	1.52
1	D	322	ASN	CG-OD1	6.71	1.36	1.23
1	F	175	THR	CB-CG2	-6.68	1.30	1.52
1	B	412[A]	ASP	C-O	6.49	1.31	1.23
1	B	412[B]	ASP	C-O	6.49	1.31	1.23
1	E	181	LEU	N-CA	-6.39	1.38	1.46
1	E	412	ASP	N-CA	-6.32	1.38	1.46
1	C	376	TYR	CA-C	-6.23	1.44	1.52
1	B	293	VAL	N-CA	6.10	1.53	1.46
1	D	412	ASP	N-CA	-5.93	1.38	1.46
1	F	332	SER	CB-OG	-5.90	1.30	1.42
1	C	304	ARG	CA-C	5.89	1.61	1.52
1	A	33	GLN	N-CA	5.84	1.53	1.46
1	B	368	GLY	CA-C	5.77	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	GLU	CA-CB	5.66	1.62	1.53
1	E	260	ARG	N-CA	-5.65	1.38	1.46
1	E	412	ASP	C-O	5.64	1.30	1.23
1	E	186	LEU	C-O	-5.57	1.17	1.24
1	F	175	THR	CA-C	-5.57	1.45	1.52
1	F	343	MET	N-CA	5.40	1.52	1.45
1	F	332	SER	C-O	-5.37	1.17	1.23
1	C	33	GLN	N-CA	5.36	1.53	1.46
1	E	94	VAL	N-CA	-5.34	1.41	1.47
1	C	304	ARG	N-CA	5.34	1.53	1.46
1	F	304	ARG	N-CA	5.33	1.53	1.46
1	E	267	LEU	CA-C	-5.30	1.46	1.52
1	F	442	GLN	N-CA	-5.25	1.39	1.46
1	B	304	ARG	N-CA	5.24	1.52	1.46
1	B	89	ASN	C-O	-5.22	1.17	1.23
1	D	52	LEU	C-O	5.18	1.30	1.23
1	C	104	ILE	C-O	-5.16	1.18	1.24
1	F	292	THR	N-CA	5.14	1.52	1.46
1	B	304	ARG	CA-C	5.10	1.59	1.52
1	F	183	ILE	N-CA	-5.08	1.39	1.46
1	B	100	ALA	CA-C	-5.08	1.48	1.52
1	C	268	VAL	C-O	-5.08	1.17	1.23
1	F	114	GLY	CA-C	-5.06	1.48	1.52
1	E	225	VAL	CA-CB	5.02	1.61	1.54
1	B	42	GLY	C-O	5.01	1.28	1.23

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	452	ARG	CG-CD-NE	6.60	126.52	112.00
1	C	251	GLU	CB-CA-C	6.47	120.38	109.84
1	F	292	THR	N-CA-C	6.22	120.57	112.92
1	D	435	ILE	N-CA-C	-6.05	104.61	110.42
1	E	300	LEU	N-CA-C	6.03	117.93	111.36
1	D	436	ASN	N-CA-C	6.00	117.90	111.36
1	F	412	ASP	N-CA-C	-5.93	101.26	110.10
1	B	339	TYR	CA-C-N	-5.92	113.66	119.76
1	B	339	TYR	C-N-CA	-5.92	113.66	119.76
1	F	175	THR	N-CA-CB	5.82	118.77	110.16
1	D	262	ARG	N-CA-C	5.68	117.92	111.11
1	B	450	TYR	N-CA-C	5.60	121.00	113.72
1	B	251	GLU	CB-CA-C	5.60	119.23	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	THR	CB-CA-C	-5.56	101.16	110.56
1	F	292	THR	CB-CA-C	-5.53	101.22	110.56
1	D	450	TYR	N-CA-C	5.46	120.82	113.72
1	E	117	PHE	CB-CA-C	5.40	115.52	110.17
1	D	350	ASN	CB-CA-C	5.33	120.36	109.55
1	C	300	LEU	N-CA-C	5.29	118.20	111.69
1	F	300	LEU	N-CA-C	5.27	118.87	112.23
1	A	143	THR	N-CA-CB	5.16	119.42	110.39
1	F	250	SER	N-CA-C	-5.14	104.80	111.74
1	A	458	LEU	CA-C-N	5.01	127.39	120.67
1	A	458	LEU	C-N-CA	5.01	127.39	120.67
1	D	294	ARG	CG-CD-NE	-5.01	100.97	112.00
1	F	323	LEU	CA-C-N	-5.01	113.88	119.19
1	F	323	LEU	C-N-CA	-5.01	113.88	119.19
1	C	235	GLY	N-CA-C	5.00	118.30	112.50
1	B	395	LEU	CB-CA-C	-5.00	99.45	109.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3360	0	3297	44	0
1	B	3281	0	3247	41	0
1	C	3240	0	3207	55	0
1	D	3192	0	3155	43	0
1	E	3221	0	3168	47	0
1	F	3264	0	3218	46	0
2	A	10	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
2	E	20	0	0	0	0
2	F	15	0	0	0	0
3	A	13	0	5	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	5	2	0
3	C	13	0	5	5	0
3	D	13	0	5	3	0
3	E	13	0	5	2	0
3	F	13	0	5	3	0
4	A	18	0	24	2	0
4	B	12	0	16	0	0
4	C	12	0	16	0	0
4	E	6	0	8	0	0
4	F	6	0	8	0	0
5	A	26	0	16	8	0
5	B	26	0	16	8	0
5	D	26	0	16	5	0
6	D	7	0	10	10	0
6	E	7	0	10	7	0
6	F	7	0	10	12	0
7	A	388	0	0	9	3
7	B	346	0	0	8	0
7	C	327	0	0	15	0
7	D	339	0	0	14	3
7	E	352	0	0	12	3
7	F	346	0	0	10	1
All	All	21977	0	19472	271	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (271) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57[A]:ARG:HH21	1:C:59[A]:GLN:NE2	1.01	1.48
1:C:57[A]:ARG:NH2	1:C:59[A]:GLN:HE22	1.08	1.47
1:B:294[A]:ARG:NH2	1:B:297:GLU:OE1	1.75	1.20
1:E:84:ARG:HD2	7:E:747:HOH:O	1.53	1.04
1:C:57[A]:ARG:NH2	1:C:59[A]:GLN:NE2	1.79	1.01
1:C:292:THR:OG1	7:C:601:HOH:O	1.71	1.00
1:D:102:MET:CE	7:D:717:HOH:O	2.11	0.96
1:D:42:GLY:N	7:D:603:HOH:O	2.00	0.93
1:D:102:MET:HE2	7:D:717:HOH:O	1.66	0.92
1:F:102[B]:MET:HE3	1:F:162:LEU:HD12	1.51	0.92
1:B:295[B]:ILE:HG22	1:B:295[B]:ILE:O	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:MET:CE	7:C:644:HOH:O	2.19	0.91
1:F:102[B]:MET:SD	7:F:834:HOH:O	2.28	0.91
1:B:427[B]:ARG:NH2	7:B:601:HOH:O	1.83	0.88
1:E:422:ARG:HE	6:E:506:PEG:H21	1.39	0.88
1:F:422:ARG:HE	6:F:505:PEG:H12	1.36	0.88
1:D:243:GLU:OE2	7:D:602:HOH:O	1.92	0.86
1:D:422:ARG:HE	6:D:505:PEG:H32	1.42	0.85
1:C:152:HIS:ND1	3:C:501:FLC:HG2	1.91	0.85
3:C:501:FLC:OB2	1:E:304:ARG:HA	1.78	0.84
1:A:294[A]:ARG:NH2	1:F:294[A]:ARG:NH1	2.27	0.82
5:A:507[A]:IAC:H171	6:F:505:PEG:H21	1.60	0.81
1:F:173:GLU:HG3	7:F:732:HOH:O	1.80	0.81
1:C:57[A]:ARG:CZ	1:C:59[A]:GLN:NE2	2.44	0.81
1:D:294:ARG:NH2	1:D:297:GLU:OE1	2.14	0.79
3:B:504:FLC:OB2	1:D:304:ARG:HA	1.82	0.79
1:F:422:ARG:HE	6:F:505:PEG:C1	1.95	0.79
1:B:102:MET:HE3	1:B:162:LEU:HD12	1.66	0.78
1:E:102:MET:CE	7:E:609:HOH:O	2.32	0.78
1:E:297:GLU:OE2	1:E:322[B]:ASN:ND2	2.16	0.78
1:F:297:GLU:OE1	1:F:322[B]:ASN:OD1	2.02	0.77
1:A:102:MET:HE3	1:A:162:LEU:HD12	1.65	0.77
5:B:506[B]:IAC:O3	6:D:505:PEG:H42	1.85	0.77
1:B:102:MET:HE1	1:B:168:HIS:CE1	2.20	0.76
1:D:327:ARG:NH1	1:D:412:ASP:OD2	2.17	0.76
1:D:422:ARG:NE	6:D:505:PEG:H32	2.01	0.76
1:B:88:GLU:OE1	1:B:260:ARG:NH2	2.18	0.75
1:A:102:MET:CE	1:A:162:LEU:HD12	2.16	0.75
1:E:304:ARG:HH21	1:E:322[B]:ASN:ND2	1.84	0.74
1:F:102[B]:MET:HE1	1:F:168:HIS:CE1	2.22	0.74
3:D:502:FLC:OHB	3:D:502:FLC:OG2	2.05	0.74
1:A:350[A]:ASN:O	7:A:601:HOH:O	2.06	0.73
1:E:304:ARG:HH21	1:E:322[B]:ASN:HD21	1.36	0.72
5:B:506[B]:IAC:C18	6:D:505:PEG:H42	2.19	0.72
1:A:294[A]:ARG:HH21	1:F:294[A]:ARG:NH1	1.87	0.72
5:A:507[A]:IAC:O3	6:F:505:PEG:H22	1.88	0.72
1:F:147:GLN:OE1	7:F:601:HOH:O	2.08	0.72
1:E:207:LYS:NZ	7:E:601:HOH:O	2.23	0.71
1:E:102:MET:HE3	7:E:609:HOH:O	1.91	0.70
1:C:350[B]:ASN:CG	7:C:620:HOH:O	2.33	0.70
1:F:327:ARG:NH1	1:F:412:ASP:OD1	2.21	0.70
6:F:505:PEG:O4	7:F:602:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322[B]:ASN:ND2	7:A:605:HOH:O	2.25	0.68
1:B:161:ALA:O	1:B:295[B]:ILE:CG2	2.41	0.68
1:A:327:ARG:NH1	1:A:412:ASP:OD2	2.25	0.68
1:B:427[B]:ARG:NE	7:B:601:HOH:O	2.25	0.67
1:F:194:ASP:HB2	7:F:696:HOH:O	1.94	0.67
1:B:160:ILE:HG23	1:B:295[A]:ILE:HG22	1.77	0.67
1:E:304:ARG:NH2	1:E:322[B]:ASN:ND2	2.42	0.67
1:D:422:ARG:HE	6:D:505:PEG:C3	2.07	0.66
1:C:161:ALA:O	1:C:295[A]:ILE:HG23	1.96	0.66
1:C:33:GLN:HA	7:C:812:HOH:O	1.95	0.66
1:C:57[A]:ARG:HE	1:C:59[A]:GLN:NE2	1.94	0.66
1:C:350[B]:ASN:O	7:C:602:HOH:O	2.09	0.66
1:D:152:HIS:ND1	3:D:502:FLC:OG2	2.27	0.66
1:F:301[B]:ASN:OD1	1:F:301[B]:ASN:O	2.15	0.65
1:B:304:ARG:HA	3:D:502:FLC:OB2	1.97	0.65
1:E:297:GLU:OE1	1:E:322[B]:ASN:OD1	2.15	0.65
1:B:317:THR:HB	7:B:630:HOH:O	1.95	0.65
5:D:506[B]:IAC:O2	6:E:506:PEG:H11	1.97	0.65
3:A:503:FLC:OB1	1:F:304:ARG:HA	1.98	0.64
1:A:102:MET:HE1	1:A:168:HIS:CE1	2.33	0.63
1:E:422:ARG:NE	6:E:506:PEG:H21	2.11	0.63
1:A:102:MET:HE3	1:A:104:ILE:HD11	1.81	0.63
1:C:57[A]:ARG:NE	1:C:59[A]:GLN:NE2	2.45	0.63
1:D:301:ASN:O	7:D:604:HOH:O	2.15	0.63
1:F:301[B]:ASN:ND2	7:F:606:HOH:O	2.30	0.63
1:B:435:ILE:CD1	1:C:143:THR:HG21	2.28	0.62
1:C:150:LYS:HE2	7:C:746:HOH:O	1.98	0.62
1:D:161:ALA:O	1:D:295:ILE:HG23	2.00	0.62
1:C:102:MET:HE3	7:C:644:HOH:O	1.92	0.62
1:E:422:ARG:HE	6:E:506:PEG:C2	2.12	0.61
1:C:82:ALA:N	7:C:612:HOH:O	2.34	0.61
1:A:297:GLU:OE1	1:A:322[B]:ASN:OD1	2.19	0.61
1:C:317:THR:OG1	7:C:603:HOH:O	2.16	0.61
1:D:119:GLY:O	5:D:506[B]:IAC:H5	2.01	0.61
1:F:350:ASN:O	7:F:603:HOH:O	2.16	0.61
1:C:57[A]:ARG:HE	1:C:59[A]:GLN:HE21	1.47	0.60
1:C:160:ILE:HG23	1:C:295[B]:ILE:HG23	1.84	0.60
1:E:295:ILE:O	1:E:295:ILE:HG22	2.00	0.59
1:A:422[A]:ARG:O	5:B:506[A]:IAC:H3	2.03	0.59
1:B:296:LYS:HE3	3:B:504:FLC:HG2	1.83	0.59
1:C:252:ASN:N	7:C:605:HOH:O	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:HIS:ND1	3:C:501:FLC:CG	2.66	0.59
1:B:161:ALA:O	1:B:295[B]:ILE:HG23	2.02	0.59
1:A:296:LYS:HG2	3:A:503:FLC:OG1	2.03	0.58
1:E:161:ALA:O	1:E:295:ILE:HG23	2.02	0.58
1:C:160:ILE:HG23	1:C:295[B]:ILE:CG2	2.33	0.58
1:D:237:ALA:O	1:E:452:ARG:HD3	2.04	0.58
1:C:296:LYS:HE3	3:C:501:FLC:HG1	1.86	0.58
1:C:422:ARG:HD2	6:F:505:PEG:H41	1.86	0.57
1:F:102[B]:MET:CE	1:F:162:LEU:HD12	2.29	0.57
5:A:507[A]:IAC:H171	6:F:505:PEG:C2	2.32	0.57
1:F:160:ILE:HG23	1:F:295[B]:ILE:CG2	2.34	0.57
1:C:290:LEU:O	1:C:293[B]:VAL:HG23	2.04	0.57
1:A:161:ALA:O	1:A:295[A]:ILE:HG23	2.05	0.56
1:C:41:ILE:O	1:C:41:ILE:HG23	2.03	0.56
1:E:354:SER:HB3	7:E:700:HOH:O	2.04	0.56
1:F:161:ALA:O	1:F:295[A]:ILE:HG23	2.05	0.56
5:B:506[B]:IAC:C18	6:D:505:PEG:C4	2.83	0.56
1:C:57[A]:ARG:NE	1:C:59[A]:GLN:HE21	2.01	0.56
1:D:304:ARG:NH2	1:D:317:THR:O	2.35	0.56
5:A:507[A]:IAC:C18	1:C:422:ARG:O	2.53	0.55
1:F:346:PRO:HB3	1:F:395:LEU:HG	1.88	0.55
1:D:42:GLY:CA	7:D:603:HOH:O	2.47	0.55
1:E:296:LYS:HG2	3:E:504:FLC:OG2	2.06	0.55
1:F:422:ARG:NE	6:F:505:PEG:C1	2.68	0.55
1:E:327:ARG:NH1	1:E:412:ASP:OD1	2.38	0.54
1:A:427[B]:ARG:NH2	7:A:602:HOH:O	2.11	0.54
1:E:322[B]:ASN:OD1	1:E:322[B]:ASN:O	2.25	0.54
1:C:382:GLN:NE2	7:C:614:HOH:O	2.40	0.54
1:C:322:ASN:O	1:E:294[A]:ARG:HD3	2.08	0.53
1:E:427[B]:ARG:NH2	7:E:602:HOH:O	2.23	0.53
1:A:90[B]:ARG:NH2	7:A:609:HOH:O	2.42	0.53
1:B:150[B]:LYS:HE2	7:B:798:HOH:O	2.08	0.53
1:F:296:LYS:HE3	3:F:501:FLC:HG2	1.91	0.53
1:B:143:THR:HG21	1:B:266:ARG:CZ	2.40	0.52
1:B:347:GLU:HB2	1:B:417:THR:O	2.09	0.52
1:B:102:MET:HE3	1:B:162:LEU:CD1	2.36	0.52
1:C:304:ARG:HA	3:E:504:FLC:OB1	2.10	0.52
1:D:206:GLN:N	7:D:612:HOH:O	2.40	0.51
1:A:175[A]:THR:HG22	4:A:506:GOL:H2	1.92	0.51
1:B:105:ILE:HD12	1:B:181:LEU:HD23	1.91	0.51
1:D:350:ASN:O	7:D:605:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:173:GLU:HB3	7:F:656:HOH:O	2.11	0.51
1:A:286[A]:TYR:CE1	1:E:290:LEU:HD21	2.46	0.51
1:A:427[B]:ARG:NE	7:A:602:HOH:O	2.40	0.51
1:A:173:GLU:HG3	7:A:620:HOH:O	2.11	0.51
1:E:422:ARG:HH21	6:E:506:PEG:H12	1.75	0.51
1:E:349:ASN:ND2	7:E:604:HOH:O	2.27	0.51
5:A:507[B]:IAC:C18	7:F:602:HOH:O	2.59	0.50
1:C:102:MET:HE2	7:C:644:HOH:O	1.96	0.50
1:C:438:PHE:HB2	1:C:440:LEU:HG	1.93	0.50
1:B:304:ARG:NH2	1:B:317:THR:O	2.44	0.50
1:D:286:TYR:HB3	1:D:290:LEU:HD23	1.94	0.50
1:A:304:ARG:NH2	1:A:322[B]:ASN:ND2	2.60	0.50
1:C:119:GLY:O	5:D:506[A]:IAC:H5	2.11	0.50
1:C:293[A]:VAL:HG13	1:C:293[A]:VAL:O	2.11	0.50
1:C:160:ILE:HG23	1:C:295[A]:ILE:HG22	1.94	0.49
1:F:57[B]:ARG:HG2	1:F:57[B]:ARG:HH11	1.77	0.49
1:B:422:ARG:O	5:D:506[B]:IAC:C18	2.61	0.49
1:E:322[B]:ASN:OD1	1:E:322[B]:ASN:C	2.54	0.49
6:D:505:PEG:O1	7:D:606:HOH:O	2.19	0.49
1:A:343:MET:HE2	1:B:233:PHE:CE1	2.48	0.49
1:D:438:PHE:HB2	1:D:440:LEU:HG	1.94	0.49
1:B:143:THR:HG21	1:B:266:ARG:NE	2.27	0.49
1:D:295:ILE:HG22	1:D:295:ILE:O	2.12	0.49
1:F:358:VAL:HG22	1:F:405:LEU:CD2	2.43	0.48
1:B:311:ARG:HD2	1:D:128:HIS:CE1	2.48	0.48
1:F:296:LYS:HG2	3:F:501:FLC:OA1	2.13	0.48
1:F:422:ARG:NE	6:F:505:PEG:H11	2.27	0.48
1:A:143:THR:HG22	1:C:442:GLN:NE2	2.29	0.48
1:C:294[A]:ARG:NH1	3:C:501:FLC:OG1	2.47	0.48
1:E:86:VAL:HG22	1:E:179:VAL:HG22	1.95	0.48
1:C:143:THR:O	1:C:143:THR:OG1	2.24	0.48
1:D:160:ILE:HG23	1:D:295:ILE:HG22	1.96	0.48
1:E:422:ARG:NH2	6:E:506:PEG:H12	2.29	0.48
5:A:507[A]:IAC:C18	6:F:505:PEG:H22	2.44	0.47
1:A:294[A]:ARG:HG3	3:A:503:FLC:CGC	2.44	0.47
1:A:176:GLU:HG2	4:A:506:GOL:O1	2.14	0.47
1:A:422[A]:ARG:NH1	1:F:125:GLN:OE1	2.48	0.47
1:A:372:LYS:HG3	1:B:227:GLN:HB3	1.97	0.47
5:B:506[B]:IAC:H5	1:F:119:GLY:O	2.14	0.47
1:F:327:ARG:HD2	1:F:412:ASP:OD1	2.14	0.47
5:A:507[B]:IAC:H2	6:F:505:PEG:H21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:603:HOH:O	1:E:292:THR:HB	2.14	0.46
5:D:506[A]:IAC:C18	7:E:617:HOH:O	2.62	0.46
1:E:207:LYS:NZ	7:E:618:HOH:O	2.48	0.46
1:B:160:ILE:HG23	1:B:295[A]:ILE:CG2	2.44	0.46
1:B:294[A]:ARG:NH1	1:D:322:ASN:O	2.49	0.46
5:B:506[A]:IAC:H171	6:D:505:PEG:H31	1.97	0.46
1:E:431:LEU:HD22	1:E:445:ALA:HB1	1.98	0.46
1:A:397:GLN:OE1	1:B:236:ARG:NH2	2.49	0.46
3:A:503:FLC:CAC	7:A:738:HOH:O	2.64	0.46
1:F:57[A]:ARG:NH2	1:F:66:GLU:OE2	2.49	0.46
1:A:267:LEU:C	1:A:267:LEU:HD12	2.41	0.46
1:A:143:THR:HG22	1:C:442:GLN:CD	2.41	0.45
1:C:90[A]:ARG:HB2	1:C:90[A]:ARG:NH1	2.31	0.45
1:C:105:ILE:HD12	1:C:181:LEU:HD23	1.99	0.45
1:E:422:ARG:HH21	6:E:506:PEG:C1	2.29	0.45
1:A:143:THR:HG23	1:A:266:ARG:NH1	2.32	0.45
1:C:304:ARG:NH2	1:C:317:THR:O	2.41	0.45
1:A:295[A]:ILE:O	1:A:295[A]:ILE:HG22	2.17	0.45
5:B:506[A]:IAC:O3	6:D:505:PEG:H11	2.17	0.45
1:E:202:LEU:N	1:E:202:LEU:HD12	2.32	0.45
1:E:160:ILE:HG23	1:E:295:ILE:HG22	1.98	0.45
1:B:388:ILE:HD13	1:B:394:TYR:CD2	2.51	0.44
1:B:425:VAL:HG21	1:C:167:VAL:HG21	1.98	0.44
1:D:96:SER:HB3	1:D:201:PHE:CD2	2.52	0.44
1:A:64:TYR:OH	7:A:603:HOH:O	2.21	0.44
1:E:92:LEU:O	1:E:258:MET:HA	2.17	0.44
1:C:128:HIS:CD2	1:E:311:ARG:HD2	2.52	0.44
1:A:119:GLY:O	5:A:507[B]:IAC:H5	2.18	0.44
1:D:263:ASP:N	7:D:601:HOH:O	1.76	0.44
1:B:102:MET:HE2	7:B:745:HOH:O	2.18	0.44
1:E:70:PRO:HB3	1:E:81[A]:ASP:OD1	2.17	0.44
1:E:304:ARG:NH2	1:E:322[B]:ASN:HD22	2.15	0.44
1:D:143:THR:HG23	1:D:266:ARG:CZ	2.48	0.44
1:B:397:GLN:OE1	1:C:236:ARG:NH1	2.51	0.44
1:C:422:ARG:CD	6:F:505:PEG:H41	2.48	0.44
1:D:388:ILE:HD13	1:D:394:TYR:CD2	2.53	0.44
1:E:427[B]:ARG:NE	7:E:602:HOH:O	2.44	0.44
1:D:390:GLN:O	1:D:391:ASN:HB2	2.18	0.43
1:A:360:ARG:NH1	7:A:624:HOH:O	2.52	0.43
1:D:143:THR:HG23	1:D:266:ARG:NH2	2.32	0.43
1:D:230:ASP:OD2	1:D:230:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:THR:O	1:D:143:THR:OG1	2.18	0.43
1:F:427[C]:ARG:NH2	7:F:630:HOH:O	2.51	0.43
1:C:143:THR:HG23	1:C:266:ARG:NH2	2.33	0.43
1:C:143:THR:HG23	1:C:266:ARG:CZ	2.47	0.43
1:C:49:VAL:HG22	1:C:375:VAL:HG12	2.01	0.43
1:E:84:ARG:CD	7:E:747:HOH:O	2.35	0.43
1:E:200:TYR:HB3	1:E:225:VAL:CG1	2.48	0.43
5:B:506[A]:IAC:C18	7:D:606:HOH:O	2.67	0.43
1:F:201:PHE:CE1	1:F:222:TRP:NE1	2.87	0.43
1:A:294[A]:ARG:NH2	1:F:294[A]:ARG:HH11	2.12	0.42
1:F:112:ILE:CD1	1:F:153:PHE:CE2	3.02	0.42
1:E:96:SER:HB3	1:E:201:PHE:CD2	2.54	0.42
1:F:265:LEU:CD2	1:F:267:LEU:HD21	2.49	0.42
1:F:431:LEU:HD22	1:F:445:ALA:HB1	2.02	0.42
1:E:231:PRO:HA	1:E:245:ILE:HG21	2.01	0.42
1:F:304:ARG:NH2	1:F:322[B]:ASN:ND2	2.67	0.42
1:D:166:ILE:N	7:D:615:HOH:O	2.52	0.42
1:A:420:VAL:CG1	1:A:452:ARG:HG3	2.49	0.42
1:A:294[A]:ARG:HH21	1:F:294[A]:ARG:HH11	1.62	0.42
1:A:438:PHE:HB2	1:A:440:LEU:HG	2.01	0.42
1:B:294[A]:ARG:NH1	1:D:294:ARG:NH2	2.68	0.42
1:B:294[A]:ARG:HH12	1:D:294:ARG:HE	1.66	0.42
1:D:422:ARG:HH21	6:D:505:PEG:C4	2.33	0.42
1:A:273:GLU:O	1:F:360:ARG:NH2	2.53	0.42
1:A:358:VAL:HG22	1:A:405:LEU:CD2	2.49	0.42
1:D:360:ARG:HB2	1:D:404:GLU:HB3	2.02	0.42
1:E:295:ILE:O	1:E:295:ILE:CG2	2.67	0.42
1:B:219:ASN:N	7:B:619:HOH:O	2.53	0.41
1:A:160:ILE:HG23	1:A:295[B]:ILE:HG23	2.03	0.41
1:B:273:GLU:O	1:D:360:ARG:NH2	2.52	0.41
1:B:70:PRO:HB3	1:B:81:ASP:OD1	2.21	0.41
1:C:346:PRO:HB3	1:C:395:LEU:HG	2.03	0.41
1:B:346:PRO:HB3	1:B:395:LEU:HG	2.03	0.41
1:B:389:PRO:HB2	1:B:392:TYR:CD1	2.56	0.41
1:B:438:PHE:HB2	1:B:440:LEU:HG	2.03	0.41
1:D:363:GLY:O	1:D:379:ASP:HA	2.21	0.41
1:F:250:SER:OG	1:F:253:ASP:HB3	2.20	0.41
1:D:28:ARG:HD2	7:E:631:HOH:O	2.20	0.41
1:D:219:ASN:N	7:D:635:HOH:O	2.54	0.41
1:F:160:ILE:HG23	1:F:295[A]:ILE:HG22	2.03	0.41
1:E:33:GLN:OE1	1:E:33:GLN:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ALA:HB1	1:A:329:LEU:HD12	2.02	0.40
1:A:294[A]:ARG:NH2	1:F:294[A]:ARG:CZ	2.83	0.40
1:B:290[B]:LEU:HD12	1:F:286:TYR:CZ	2.56	0.40
7:C:603:HOH:O	1:E:292:THR:CB	2.68	0.40
1:C:350[B]:ASN:ND2	7:C:620:HOH:O	2.48	0.40
1:F:295[B]:ILE:O	1:F:295[B]:ILE:HG23	2.22	0.40
1:A:33:GLN:HB3	1:A:76:GLN:HE22	1.86	0.40
1:C:303:GLU:HB3	1:E:153:PHE:CD1	2.56	0.40
3:F:501:FLC:OG1	3:F:501:FLC:OHB	2.39	0.40
1:D:41:ILE:HG13	7:D:603:HOH:O	2.21	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:746:HOH:O	7:E:883:HOH:O[4_556]	1.46	0.74
7:A:868:HOH:O	7:F:750:HOH:O[3_545]	1.58	0.62
7:D:858:HOH:O	7:E:883:HOH:O[4_556]	1.94	0.26
7:A:898:HOH:O	7:E:651:HOH:O[2_454]	2.08	0.12
7:A:898:HOH:O	7:D:601:HOH:O[2_454]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	409/479 (85%)	393 (96%)	16 (4%)	0	100	100
1	B	359/479 (75%)	344 (96%)	14 (4%)	1 (0%)	36	22
1	C	317/479 (66%)	305 (96%)	12 (4%)	0	100	100
1	D	390/479 (81%)	378 (97%)	12 (3%)	0	100	100
1	E	393/479 (82%)	378 (96%)	13 (3%)	2 (0%)	24	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	398/479 (83%)	382 (96%)	16 (4%)	0	100	100
All	All	2266/2874 (79%)	2180 (96%)	83 (4%)	3 (0%)	48	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	41	ILE
1	B	33	GLN
1	E	193	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/416 (89%)	361 (98%)	8 (2%)	45	29
1	B	362/416 (87%)	352 (97%)	10 (3%)	38	21
1	C	356/416 (86%)	344 (97%)	12 (3%)	32	16
1	D	350/416 (84%)	344 (98%)	6 (2%)	53	38
1	E	353/416 (85%)	346 (98%)	7 (2%)	48	32
1	F	358/416 (86%)	352 (98%)	6 (2%)	53	38
All	All	2148/2496 (86%)	2099 (98%)	49 (2%)	47	27

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	130	THR
1	A	143	THR
1	A	173	GLU
1	A	269	ARG
1	A	371[A]	SER
1	A	371[B]	SER
1	A	431	LEU

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Mol	Chain	Res	Type
1	B	33	GLN
1	B	76	GLN
1	B	206	GLN
1	B	251	GLU
1	B	269	ARG
1	B	350[A]	ASN
1	B	350[B]	ASN
1	B	371	SER
1	B	381	ARG
1	B	461	GLU
1	C	33	GLN
1	C	41	ILE
1	C	50	ASN
1	C	80	ILE
1	C	81	ASP
1	C	90[A]	ARG
1	C	90[B]	ARG
1	C	175	THR
1	C	294[A]	ARG
1	C	294[B]	ARG
1	C	427[A]	ARG
1	C	427[B]	ARG
1	D	72	SER
1	D	88	GLU
1	D	130	THR
1	D	243	GLU
1	D	290	LEU
1	D	360	ARG
1	E	33	GLN
1	E	80	ILE
1	E	175	THR
1	E	269	ARG
1	E	354	SER
1	E	371	SER
1	E	452	ARG
1	F	34	SER
1	F	173	GLU
1	F	175	THR
1	F	206	GLN
1	F	354	SER
1	F	431	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	330	GLN
1	A	382	GLN
1	B	76	GLN
1	B	142	GLN
1	B	196	ASN
1	B	223	ASN
1	B	249	GLN
1	B	391	ASN
1	C	147	GLN
1	C	382	GLN
1	C	401	GLN
1	C	439	GLN
1	D	128	HIS
1	D	223	ASN
1	D	227	GLN
1	D	249	GLN
1	D	391	ASN
1	D	401	GLN
1	E	147	GLN
1	E	219	ASN
1	E	391	ASN
1	F	50	ASN
1	F	350	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

42 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	C	506	-	4,4,4	0.90	0	6,6,6	0.36	0
2	PO4	E	505	-	4,4,4	0.75	0	6,6,6	1.15	1 (16%)
3	FLC	F	501	-	12,12,12	1.87	3 (25%)	17,17,17	5.74	11 (64%)
4	GOL	A	504	-	5,5,5	0.38	0	5,5,5	0.50	0
5	IAC	B	506[B]	-	14,14,14	1.78	2 (14%)	19,19,19	1.49	2 (10%)
2	PO4	F	504	-	4,4,4	1.16	0	6,6,6	1.63	1 (16%)
6	PEG	E	506	-	6,6,6	0.86	0	5,5,5	1.17	0
4	GOL	C	502	-	5,5,5	0.64	0	5,5,5	0.77	0
3	FLC	D	502	-	12,12,12	1.62	2 (16%)	17,17,17	4.39	9 (52%)
5	IAC	D	506[B]	-	14,14,14	2.02	3 (21%)	19,19,19	1.81	4 (21%)
2	PO4	E	502	-	4,4,4	1.35	0	6,6,6	1.11	1 (16%)
6	PEG	D	505	-	6,6,6	0.97	0	5,5,5	1.90	3 (60%)
4	GOL	F	506	-	5,5,5	0.88	0	5,5,5	0.81	0
2	PO4	C	505	-	4,4,4	1.33	0	6,6,6	2.10	3 (50%)
4	GOL	C	503	-	5,5,5	0.61	0	5,5,5	0.85	0
2	PO4	F	502	-	4,4,4	1.09	0	6,6,6	1.39	1 (16%)
3	FLC	C	501	-	12,12,12	1.79	1 (8%)	17,17,17	4.62	12 (70%)
2	PO4	D	501	-	4,4,4	0.80	0	6,6,6	1.77	2 (33%)
4	GOL	E	503	-	5,5,5	0.55	0	5,5,5	0.65	0
2	PO4	B	502	-	4,4,4	0.96	0	6,6,6	1.76	1 (16%)
5	IAC	B	506[A]	-	14,14,14	1.87	2 (14%)	19,19,19	2.01	4 (21%)
2	PO4	C	504	-	4,4,4	0.95	0	6,6,6	1.18	0
2	PO4	E	507	-	4,4,4	0.83	0	6,6,6	0.62	0
4	GOL	B	503	-	5,5,5	1.69	2 (40%)	5,5,5	1.80	2 (40%)
5	IAC	D	506[A]	-	14,14,14	2.09	3 (21%)	19,19,19	1.44	4 (21%)
2	PO4	A	501	-	4,4,4	1.38	1 (25%)	6,6,6	1.33	0
4	GOL	A	505	-	5,5,5	0.69	0	5,5,5	0.55	0
5	IAC	A	507[B]	-	14,14,14	2.02	4 (28%)	19,19,19	1.87	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	B	505	-	4,4,4	1.00	0	6,6,6	2.08	2 (33%)
3	FLC	E	504	-	12,12,12	1.43	2 (16%)	17,17,17	4.86	11 (64%)
2	PO4	E	501	-	4,4,4	1.28	1 (25%)	6,6,6	1.63	2 (33%)
4	GOL	B	507	-	5,5,5	0.90	0	5,5,5	0.67	0
4	GOL	A	506	-	5,5,5	0.52	0	5,5,5	0.37	0
3	FLC	B	504	-	12,12,12	1.98	5 (41%)	17,17,17	5.41	10 (58%)
3	FLC	A	503	-	12,12,12	1.71	3 (25%)	17,17,17	4.79	12 (70%)
2	PO4	A	502	-	4,4,4	0.45	0	6,6,6	1.35	1 (16%)
2	PO4	D	504	-	4,4,4	0.77	0	6,6,6	0.80	0
5	IAC	A	507[A]	-	14,14,14	2.20	5 (35%)	19,19,19	2.02	6 (31%)
2	PO4	B	501	-	4,4,4	2.41	1 (25%)	6,6,6	2.53	3 (50%)
2	PO4	F	503	-	4,4,4	0.96	0	6,6,6	1.97	2 (33%)
2	PO4	D	503	-	4,4,4	0.91	0	6,6,6	0.42	0
6	PEG	F	505	-	6,6,6	1.09	1 (16%)	5,5,5	2.13	2 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FLC	F	501	-	-	11/16/16/16	-
4	GOL	A	504	-	-	1/4/4/4	-
5	IAC	B	506[B]	-	-	2/4/4/4	0/2/2/2
6	PEG	E	506	-	-	3/4/4/4	-
4	GOL	C	502	-	-	2/4/4/4	-
3	FLC	D	502	-	-	10/16/16/16	-
5	IAC	D	506[B]	-	-	2/4/4/4	0/2/2/2
6	PEG	D	505	-	-	2/4/4/4	-
4	GOL	F	506	-	-	2/4/4/4	-
4	GOL	C	503	-	-	4/4/4/4	-
3	FLC	C	501	-	-	6/16/16/16	-
4	GOL	E	503	-	-	3/4/4/4	-
5	IAC	B	506[A]	-	-	4/4/4/4	0/2/2/2
4	GOL	B	503	-	-	4/4/4/4	-
5	IAC	D	506[A]	-	-	2/4/4/4	0/2/2/2
4	GOL	A	505	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IAC	A	507[B]	-	-	2/4/4/4	0/2/2/2
3	FLC	E	504	-	-	8/16/16/16	-
4	GOL	B	507	-	-	2/4/4/4	-
4	GOL	A	506	-	-	2/4/4/4	-
3	FLC	B	504	-	-	9/16/16/16	-
3	FLC	A	503	-	-	13/16/16/16	-
5	IAC	A	507[A]	-	-	4/4/4/4	0/2/2/2
6	PEG	F	505	-	-	1/4/4/4	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	506[A]	IAC	C1-C	5.39	1.48	1.41
5	B	506[A]	IAC	C1-C	5.19	1.47	1.41
2	B	501	PO4	P-O1	4.73	1.61	1.50
5	A	507[B]	IAC	C1-C	4.63	1.47	1.41
5	A	507[A]	IAC	C1-C	4.63	1.47	1.41
5	B	506[B]	IAC	C1-C	4.43	1.46	1.41
5	D	506[B]	IAC	C1-C	4.41	1.46	1.41
3	C	501	FLC	OHB-CB	4.36	1.51	1.43
3	D	502	FLC	OHB-CB	4.03	1.50	1.43
5	D	506[B]	IAC	C1-C7	3.67	1.50	1.44
5	A	507[A]	IAC	C1-C7	3.49	1.49	1.44
3	F	501	FLC	CG-CB	3.46	1.58	1.54
3	A	503	FLC	CG-CB	-3.39	1.49	1.54
3	B	504	FLC	OHB-CB	3.33	1.49	1.43
5	D	506[A]	IAC	C-N	-3.19	1.32	1.37
3	B	504	FLC	CB-CBC	3.11	1.56	1.53
5	D	506[B]	IAC	C-N	-3.08	1.32	1.37
5	A	507[B]	IAC	C-N	-3.06	1.32	1.37
5	A	507[B]	IAC	C1-C7	2.84	1.48	1.44
3	F	501	FLC	CB-CBC	-2.75	1.50	1.53
5	A	507[A]	IAC	O2-C18	-2.74	1.21	1.30
3	E	504	FLC	OHB-CB	2.74	1.48	1.43
5	A	507[A]	IAC	C-N	-2.66	1.33	1.37
3	B	504	FLC	OG1-CGC	2.66	1.30	1.22
5	B	506[B]	IAC	C-N	-2.57	1.33	1.37
3	A	503	FLC	CB-CBC	-2.49	1.50	1.53
5	A	507[A]	IAC	C17-C18	2.48	1.54	1.51
3	B	504	FLC	CG-CB	2.43	1.57	1.54
4	B	503	GOL	C1-C2	2.38	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	FLC	CG-CGC	2.38	1.57	1.50
3	B	504	FLC	OA1-CAC	2.35	1.29	1.22
5	B	506[A]	IAC	C8-C7	2.32	1.40	1.36
3	F	501	FLC	OG1-CGC	2.30	1.29	1.22
6	F	505	PEG	O1-C1	2.21	1.53	1.42
3	D	502	FLC	OB1-CBC	2.20	1.29	1.22
2	E	501	PO4	P-O1	2.15	1.55	1.50
2	A	501	PO4	P-O1	2.14	1.55	1.50
3	E	504	FLC	CB-CBC	-2.08	1.51	1.53
4	B	503	GOL	O1-C1	2.04	1.51	1.42
5	A	507[B]	IAC	C8-C7	2.02	1.39	1.36
5	D	506[A]	IAC	C5-C	-2.00	1.36	1.39

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	501	FLC	OHB-CB-CBC	-15.90	86.40	108.96
3	B	504	FLC	OHB-CB-CG	-12.72	80.36	109.38
3	B	504	FLC	OHB-CB-CBC	-12.65	91.02	108.96
3	E	504	FLC	OHB-CB-CBC	-12.56	91.15	108.96
3	A	503	FLC	CG-CB-CA	10.62	136.57	109.31
3	A	503	FLC	OHB-CB-CA	-10.40	85.67	109.38
3	D	502	FLC	OHB-CB-CA	-9.60	87.49	109.38
3	D	502	FLC	OHB-CB-CBC	-9.17	95.95	108.96
3	C	501	FLC	OHB-CB-CA	-9.08	88.67	109.38
3	F	501	FLC	OHB-CB-CA	-8.84	89.22	109.38
3	C	501	FLC	OHB-CB-CG	-8.72	89.49	109.38
3	F	501	FLC	OHB-CB-CG	-8.55	89.88	109.38
3	C	501	FLC	CG-CB-CA	8.45	131.00	109.31
3	E	504	FLC	OHB-CB-CA	-8.14	90.81	109.38
3	B	504	FLC	CG-CB-CBC	7.91	127.53	110.03
3	E	504	FLC	OHB-CB-CG	-7.76	91.67	109.38
3	F	501	FLC	CG-CB-CBC	7.21	125.98	110.03
3	D	502	FLC	OHB-CB-CG	-6.90	93.65	109.38
3	A	503	FLC	OG2-CGC-CG	6.38	134.55	114.35
3	B	504	FLC	OHB-CB-CA	-6.32	94.97	109.38
3	D	502	FLC	CG-CB-CA	6.16	125.11	109.31
3	F	501	FLC	OB1-CBC-CB	-5.66	111.12	122.09
5	B	506[A]	IAC	C5-C-C1	-5.65	116.72	122.19
3	E	504	FLC	CA-CB-CBC	5.26	121.66	110.03
3	C	501	FLC	OHB-CB-CBC	-5.22	101.55	108.96
3	C	501	FLC	OB2-CBC-CB	5.18	123.07	113.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	FLC	CA-CB-CBC	5.18	121.49	110.03
3	A	503	FLC	OB2-CBC-CB	4.92	122.57	113.14
3	A	503	FLC	OG1-CGC-CG	-4.82	109.31	122.95
3	F	501	FLC	CG-CB-CA	4.60	121.10	109.31
5	A	507[A]	IAC	C17-C7-C1	4.59	132.41	126.43
3	B	504	FLC	OB2-CBC-CB	4.56	121.89	113.14
3	A	503	FLC	OHB-CB-CG	-4.35	99.47	109.38
3	E	504	FLC	CB-CG-CGC	4.34	125.78	113.92
3	E	504	FLC	CG-CB-CBC	4.26	119.46	110.03
3	C	501	FLC	CA-CB-CBC	4.12	119.15	110.03
5	D	506[B]	IAC	C17-C7-C1	4.06	131.72	126.43
5	B	506[B]	IAC	C5-C-C1	-4.00	118.32	122.19
3	C	501	FLC	CB-CA-CAC	3.97	124.77	113.92
2	B	501	PO4	O3-P-O2	-3.97	95.57	107.91
3	F	501	FLC	CB-CA-CAC	-3.92	103.19	113.92
5	B	506[A]	IAC	C2-C1-C	3.83	122.81	118.84
5	A	507[B]	IAC	C17-C7-C1	3.78	131.35	126.43
5	A	507[B]	IAC	C5-C-C1	-3.77	118.54	122.19
3	E	504	FLC	CG-CB-CA	3.68	118.75	109.31
6	F	505	PEG	O2-C2-C1	3.63	126.13	110.11
3	D	502	FLC	OA1-CAC-CA	-3.52	112.99	122.95
3	C	501	FLC	OG1-CGC-CG	-3.51	113.00	122.95
3	B	504	FLC	OG2-CGC-OG1	3.50	132.34	123.33
3	A	503	FLC	CA-CB-CBC	3.48	117.74	110.03
2	F	503	PO4	O2-P-O1	-3.46	98.73	110.95
5	A	507[A]	IAC	C17-C7-C8	-3.40	122.19	126.84
3	D	502	FLC	OB2-CBC-CB	3.39	119.65	113.14
3	B	504	FLC	CA-CB-CBC	3.37	117.48	110.03
3	A	503	FLC	OHB-CB-CBC	-3.36	104.19	108.96
3	C	501	FLC	OG2-CGC-CG	3.33	124.90	114.35
5	D	506[B]	IAC	C5-C-C1	-3.33	118.97	122.19
3	A	503	FLC	CG-CB-CBC	-3.25	102.84	110.03
5	A	507[B]	IAC	C-C1-C7	-3.17	103.96	107.17
2	B	505	PO4	O3-P-O2	-3.17	98.05	107.91
2	B	502	PO4	O3-P-O1	-3.17	99.75	110.95
2	B	505	PO4	O4-P-O3	3.17	117.76	107.91
5	A	507[A]	IAC	C5-C-C1	-3.13	119.16	122.19
3	E	504	FLC	OB2-CBC-CB	3.07	119.02	113.14
2	C	505	PO4	O3-P-O1	3.02	121.61	110.95
2	F	504	PO4	O4-P-O3	3.00	117.26	107.91
2	B	501	PO4	O2-P-O1	2.98	121.47	110.95
3	F	501	FLC	CB-CG-CGC	2.92	121.91	113.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	504	FLC	OA1-CAC-CA	-2.92	114.68	122.95
5	D	506[A]	IAC	C5-C-C1	-2.90	119.38	122.19
2	B	501	PO4	O4-P-O3	-2.90	98.89	107.91
6	F	505	PEG	O1-C1-C2	2.89	128.85	111.82
5	A	507[A]	IAC	C-N-C8	2.86	111.62	109.08
3	B	504	FLC	OB2-CBC-OB1	-2.83	114.79	123.86
3	A	503	FLC	OG2-CGC-OG1	-2.81	116.10	123.33
2	C	505	PO4	O2-P-O1	-2.77	101.17	110.95
5	B	506[A]	IAC	C-C1-C7	-2.73	104.41	107.17
5	A	507[A]	IAC	C-C1-C7	-2.68	104.46	107.17
5	D	506[B]	IAC	C-C1-C7	-2.68	104.46	107.17
2	C	505	PO4	O4-P-O2	-2.65	99.65	107.91
3	C	501	FLC	OA2-CAC-CA	2.62	122.66	114.35
2	D	501	PO4	O4-P-O1	-2.60	101.75	110.95
3	F	501	FLC	OB2-CBC-CB	2.58	118.09	113.14
5	A	507[B]	IAC	C17-C7-C8	-2.57	123.32	126.84
3	E	504	FLC	OG2-CGC-OG1	-2.55	116.77	123.33
2	E	501	PO4	O4-P-O2	-2.54	100.02	107.91
3	B	504	FLC	OG1-CGC-CG	-2.54	115.77	122.95
3	A	503	FLC	OB1-CBC-CB	-2.50	117.25	122.09
3	C	501	FLC	OA1-CAC-CA	-2.49	115.91	122.95
5	D	506[A]	IAC	O2-C18-O3	-2.46	117.01	123.33
4	B	503	GOL	C3-C2-C1	2.43	120.70	111.80
5	D	506[A]	IAC	O2-C18-C17	2.42	122.00	114.51
6	D	505	PEG	O1-C1-C2	2.41	125.99	111.82
5	A	507[A]	IAC	O2-C18-O3	-2.40	117.15	123.33
5	D	506[A]	IAC	C-C1-C7	-2.34	104.81	107.17
2	D	501	PO4	O4-P-O2	2.33	115.17	107.91
3	C	501	FLC	OB1-CBC-CB	-2.30	117.64	122.09
5	B	506[A]	IAC	C5-C-N	2.30	134.42	130.74
6	D	505	PEG	O2-C2-C1	2.30	120.23	110.11
3	F	501	FLC	OA2-CAC-CA	2.29	121.60	114.35
3	A	503	FLC	OA2-CAC-CA	2.25	121.47	114.35
6	D	505	PEG	O2-C3-C4	2.24	120.00	110.11
3	E	504	FLC	OG1-CGC-CG	2.24	129.29	122.95
2	E	505	PO4	O3-P-O2	2.21	114.78	107.91
3	D	502	FLC	OB1-CBC-CB	-2.20	117.83	122.09
2	E	502	PO4	O4-P-O2	2.19	114.73	107.91
3	D	502	FLC	OA2-CAC-OA1	2.18	128.94	123.33
5	D	506[B]	IAC	C17-C7-C8	-2.17	123.87	126.84
2	A	502	PO4	O4-P-O2	2.17	114.65	107.91
3	F	501	FLC	OB2-CBC-OB1	2.16	130.78	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	504	FLC	CG-CB-CA	2.14	114.81	109.31
2	F	503	PO4	O4-P-O3	2.12	114.52	107.91
4	B	503	GOL	O1-C1-C2	2.12	119.91	110.38
5	B	506[B]	IAC	C5-C-N	2.09	134.09	130.74
5	A	507[B]	IAC	C-N-C8	2.08	110.93	109.08
2	E	501	PO4	O4-P-O3	2.08	114.37	107.91
2	F	502	PO4	O4-P-O2	2.05	114.30	107.91

There are no chirality outliers.

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	FLC	CA-CB-CBC-OB1
3	A	503	FLC	CA-CB-CBC-OB2
3	A	503	FLC	OHB-CB-CBC-OB1
3	A	503	FLC	OHB-CB-CBC-OB2
3	A	503	FLC	CA-CB-CG-CGC
3	B	504	FLC	CA-CB-CBC-OB1
3	B	504	FLC	CA-CB-CBC-OB2
3	B	504	FLC	CG-CB-CBC-OB1
3	B	504	FLC	CG-CB-CBC-OB2
3	B	504	FLC	OHB-CB-CBC-OB1
3	B	504	FLC	OHB-CB-CBC-OB2
3	C	501	FLC	OHB-CB-CBC-OB1
3	C	501	FLC	OHB-CB-CBC-OB2
3	D	502	FLC	CA-CB-CBC-OB2
3	D	502	FLC	CG-CB-CBC-OB1
3	D	502	FLC	CG-CB-CBC-OB2
3	D	502	FLC	OHB-CB-CBC-OB1
3	D	502	FLC	OHB-CB-CBC-OB2
3	E	504	FLC	CA-CB-CBC-OB1
3	E	504	FLC	CA-CB-CBC-OB2
3	E	504	FLC	CG-CB-CBC-OB1
3	E	504	FLC	CG-CB-CBC-OB2
3	E	504	FLC	OHB-CB-CBC-OB1
3	E	504	FLC	OHB-CB-CBC-OB2
3	F	501	FLC	CAC-CA-CB-CBC
3	F	501	FLC	CA-CB-CBC-OB1
3	F	501	FLC	CA-CB-CBC-OB2
3	F	501	FLC	CG-CB-CBC-OB1
3	F	501	FLC	CG-CB-CBC-OB2
3	F	501	FLC	OHB-CB-CBC-OB1

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Mol	Chain	Res	Type	Atoms
3	F	501	FLC	OHB-CB-CBC-OB2
3	F	501	FLC	CA-CB-CG-CGC
4	A	505	GOL	O1-C1-C2-O2
4	A	505	GOL	O1-C1-C2-C3
4	B	503	GOL	O1-C1-C2-C3
4	B	503	GOL	C1-C2-C3-O3
4	B	507	GOL	C1-C2-C3-O3
4	C	502	GOL	C1-C2-C3-O3
4	C	503	GOL	O1-C1-C2-C3
4	F	506	GOL	O1-C1-C2-C3
5	A	507[A]	IAC	C18-C17-C7-C1
5	A	507[A]	IAC	C18-C17-C7-C8
5	A	507[B]	IAC	C18-C17-C7-C1
5	D	506[B]	IAC	C18-C17-C7-C1
3	D	502	FLC	CA-CB-CG-CGC
3	E	504	FLC	CA-CB-CG-CGC
4	A	506	GOL	O1-C1-C2-O2
6	D	505	PEG	O2-C3-C4-O4
6	E	506	PEG	O1-C1-C2-O2
3	A	503	FLC	OHB-CB-CG-CGC
3	B	504	FLC	CAC-CA-CB-CG
3	B	504	FLC	CBC-CB-CG-CGC
3	B	504	FLC	OHB-CB-CG-CGC
3	C	501	FLC	CA-CB-CG-CGC
3	F	501	FLC	OHB-CB-CG-CGC
4	A	504	GOL	C1-C2-C3-O3
4	A	505	GOL	C1-C2-C3-O3
4	A	506	GOL	O1-C1-C2-C3
4	C	503	GOL	C1-C2-C3-O3
4	E	503	GOL	C1-C2-C3-O3
6	F	505	PEG	O2-C3-C4-O4
3	A	503	FLC	CG-CB-CBC-OB2
4	B	507	GOL	O2-C2-C3-O3
4	C	502	GOL	O2-C2-C3-O3
4	C	503	GOL	O1-C1-C2-O2
5	B	506[A]	IAC	C18-C17-C7-C1
5	B	506[B]	IAC	C18-C17-C7-C1
5	D	506[A]	IAC	C18-C17-C7-C1
5	A	507[B]	IAC	C18-C17-C7-C8
5	B	506[A]	IAC	C18-C17-C7-C8
5	B	506[B]	IAC	C18-C17-C7-C8
5	D	506[A]	IAC	C18-C17-C7-C8

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Mol	Chain	Res	Type	Atoms
5	D	506[B]	IAC	C18-C17-C7-C8
3	C	501	FLC	CAC-CA-CB-CG
3	D	502	FLC	OHB-CB-CG-CGC
4	B	503	GOL	O1-C1-C2-O2
4	B	503	GOL	O2-C2-C3-O3
4	F	506	GOL	O1-C1-C2-O2
3	A	503	FLC	CAC-CA-CB-CG
3	E	504	FLC	CAC-CA-CB-CBC
3	D	502	FLC	CA-CB-CBC-OB1
4	A	505	GOL	O2-C2-C3-O3
6	D	505	PEG	O1-C1-C2-O2
4	C	503	GOL	O2-C2-C3-O3
4	E	503	GOL	O1-C1-C2-O2
4	E	503	GOL	O2-C2-C3-O3
6	E	506	PEG	O2-C3-C4-O4
3	A	503	FLC	CAC-CA-CB-OHB
3	C	501	FLC	OHB-CB-CG-CGC
6	E	506	PEG	C1-C2-O2-C3
5	A	507[A]	IAC	C7-C17-C18-O2
5	B	506[A]	IAC	C7-C17-C18-O2
3	D	502	FLC	CAC-CA-CB-CG
5	A	507[A]	IAC	C7-C17-C18-O3
5	B	506[A]	IAC	C7-C17-C18-O3
3	D	502	FLC	CAC-CA-CB-CBC
3	F	501	FLC	CAC-CA-CB-OHB
3	A	503	FLC	CBC-CB-CG-CGC
3	F	501	FLC	CAC-CA-CB-CG
3	A	503	FLC	CB-CA-CAC-OA2
3	A	503	FLC	CB-CA-CAC-OA1
3	A	503	FLC	CB-CG-CGC-OG1
3	C	501	FLC	CB-CA-CAC-OA1

There are no ring outliers.

16 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	501	FLC	3	0
5	B	506[B]	IAC	4	0
6	E	506	PEG	7	0
3	D	502	FLC	3	0
5	D	506[B]	IAC	3	0
6	D	505	PEG	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	FLC	5	0
5	B	506[A]	IAC	4	0
5	D	506[A]	IAC	2	0
5	A	507[B]	IAC	3	0
3	E	504	FLC	2	0
4	A	506	GOL	2	0
3	B	504	FLC	2	0
3	A	503	FLC	4	0
5	A	507[A]	IAC	5	0
6	F	505	PEG	12	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	399/479 (83%)	0.06	6 (1%) 72 76	7, 21, 42, 69	20 (5%)
1	B	400/479 (83%)	0.20	13 (3%) 49 53	10, 23, 50, 85	12 (3%)
1	C	397/479 (82%)	0.22	9 (2%) 61 65	11, 24, 47, 75	9 (2%)
1	D	396/479 (82%)	0.18	12 (3%) 52 56	10, 23, 42, 98	4 (1%)
1	E	397/479 (82%)	0.16	11 (2%) 55 59	10, 23, 49, 75	6 (1%)
1	F	398/479 (83%)	0.16	7 (1%) 67 72	9, 22, 47, 77	10 (2%)
All	All	2387/2874 (83%)	0.16	58 (2%) 59 64	7, 23, 46, 98	61 (2%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	41	ILE	7.3
1	A	41	ILE	7.2
1	C	41	ILE	5.2
1	D	144	PHE	4.5
1	E	144	PHE	4.3
1	E	40	GLY	4.1
1	B	41	ILE	4.1
1	D	130	THR	3.9
1	A	40	GLY	3.8
1	F	40	GLY	3.7
1	D	272	SER	3.6
1	B	462	LEU	3.5
1	A	34	SER	3.4
1	B	144	PHE	3.4
1	F	41	ILE	3.3
1	C	129	PRO	3.2
1	F	144	PHE	3.2
1	A	130	THR	3.2
1	C	40	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	144	PHE	3.1
1	E	130	THR	3.0
1	C	302	PRO	3.0
1	D	34	SER	2.9
1	D	143	THR	2.8
1	B	143	THR	2.8
1	E	41	ILE	2.7
1	E	128	HIS	2.6
1	D	129	PRO	2.6
1	E	129	PRO	2.6
1	D	395	LEU	2.5
1	F	462	LEU	2.5
1	F	242	SER	2.5
1	A	286[A]	TYR	2.5
1	B	130	THR	2.5
1	C	175	THR	2.5
1	F	143	THR	2.5
1	B	142	GLN	2.4
1	B	40	GLY	2.4
1	B	220	LEU	2.4
1	C	130	THR	2.4
1	E	206	GLN	2.4
1	D	219	ASN	2.4
1	F	252	ASN	2.4
1	C	286	TYR	2.4
1	B	292	THR	2.3
1	D	50	ASN	2.3
1	B	129	PRO	2.3
1	B	286	TYR	2.3
1	E	143	THR	2.3
1	E	219	ASN	2.3
1	E	34	SER	2.2
1	E	461	GLU	2.2
1	A	372	LYS	2.2
1	D	128	HIS	2.1
1	B	302	PRO	2.1
1	C	206	GLN	2.1
1	D	302	PRO	2.1
1	B	128	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	506	6/6	0.67	0.17	49,61,63,67	0
3	FLC	E	504	13/13	0.69	0.22	44,66,83,95	0
2	PO4	D	504	5/5	0.69	0.16	89,98,102,102	0
3	FLC	A	503	13/13	0.70	0.18	33,59,82,87	0
4	GOL	C	502	6/6	0.71	0.13	37,56,59,67	0
4	GOL	B	503	6/6	0.73	0.20	40,55,58,58	0
2	PO4	C	506	5/5	0.73	0.14	101,107,122,124	0
2	PO4	E	507	5/5	0.75	0.15	76,78,99,101	0
2	PO4	D	503	5/5	0.76	0.17	100,101,114,121	0
4	GOL	F	506	6/6	0.76	0.12	39,52,54,55	0
3	FLC	B	504	13/13	0.78	0.17	36,57,68,79	0
4	GOL	A	505	6/6	0.78	0.14	45,51,60,62	0
3	FLC	D	502	13/13	0.78	0.17	31,51,68,74	0
3	FLC	F	501	13/13	0.80	0.15	37,55,63,78	0
6	PEG	D	505	7/7	0.80	0.13	35,36,44,44	0
6	PEG	E	506	7/7	0.80	0.17	28,38,44,46	0
4	GOL	B	507	6/6	0.82	0.13	34,49,51,51	0
4	GOL	C	503	6/6	0.84	0.18	43,54,66,73	0
3	FLC	C	501	13/13	0.87	0.15	33,51,67,67	0
5	IAC	B	506[B]	13/13	0.88	0.08	21,21,22,22	13
2	PO4	F	504	5/5	0.88	0.11	45,46,54,55	0
5	IAC	B	506[A]	13/13	0.88	0.08	21,23,25,26	13
4	GOL	E	503	6/6	0.89	0.12	47,50,53,54	0
2	PO4	B	501	5/5	0.89	0.11	26,35,45,48	0
2	PO4	E	505	5/5	0.89	0.15	68,86,92,93	0
2	PO4	C	505	5/5	0.90	0.09	33,42,48,50	0
4	GOL	A	504	6/6	0.90	0.14	35,47,50,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PEG	F	505	7/7	0.91	0.11	28,34,41,42	0
2	PO4	E	501	5/5	0.92	0.10	32,39,45,51	0
5	IAC	A	507[A]	13/13	0.92	0.09	20,21,24,29	13
5	IAC	A	507[B]	13/13	0.92	0.09	23,24,29,32	13
2	PO4	D	501	5/5	0.92	0.09	34,35,46,46	0
2	PO4	F	503	5/5	0.93	0.09	34,42,44,45	0
2	PO4	F	502	5/5	0.93	0.09	35,37,47,47	0
2	PO4	C	504	5/5	0.94	0.07	35,36,47,48	0
2	PO4	A	502	5/5	0.94	0.09	34,34,41,43	0
2	PO4	E	502	5/5	0.95	0.07	35,39,44,47	0
5	IAC	D	506[A]	13/13	0.95	0.06	20,20,22,26	13
5	IAC	D	506[B]	13/13	0.95	0.06	19,20,23,23	13
2	PO4	B	502	5/5	0.95	0.07	30,32,40,43	0
2	PO4	B	505	5/5	0.95	0.08	37,38,45,52	0
2	PO4	A	501	5/5	0.95	0.10	30,33,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.